SOFTWARE FOR THE ANALYSIS OF GIANT RAMAN SCATTERING SPECTRA

Shved E. I.

Belarusian State University of Informatics and Radioelectronics
Minsk, Republic of Belarus

Bondarenko H. V. – PhD, Associate professor

There is a growing need to analyze and process giant Raman spectra for forensic and medical applications. The software is based on a database of SCR molecules adsorbed on the surface of SCR-active substrates based on silver porous silicon. The required software will facilitate the practical application of the GRS spectroscopy method and for solving applied problems.

Raman spectroscopy is based on the ability of the studied molecules to scatter monochromatic light inelastically. Raman spectroscopy allows precise identification of many molecules, but is extremely insensitive to low concentrations of chemical compounds due to the small cross-section of Raman scattering.

The effect of giant Raman scattering, which is achieved by using nanostructure substrates of noble metals, solves this problem. For molecules adsorbed on the surface of such substrates, the signal of Raman scattering is repeatedly amplified due to the localization of surface plasmons in metal nanoparticles. Existing solutions for spectra storage were analyzed, as well as the data obtained as a result of registration of GRS-spectra of different molecules. Technologies were selected for the development of the spectrum base, which will be maintained for a long time.

To create the spectra database, the data obtained by using silver-plated porous silicon as a GRS-active substrates, which were provided as text files from the confocal microscope. A drop of solution with the analyzed molecules was applied to the substrate and then the spectra were recorded by the Confotec NR500 3D scanning confocal Raman microscope. The set of the obtained spectra was provided by the supervisor.

Several variants of classifiers for the verification of the reference spectrum belonging to the considered one were examined.

Neural networks with a direct connection are universal means of functions approximation that allows to use them in the solution of classification problems. It is not known what kind of complexity the network may be required for a sufficiently accurate implementation. The Bayesian classifier was also considered during the analysis of the problem. The advantage of the Bayesian classifier is the small amount of data for training needed for the evaluation of parameters required for classification. The disadvantage is a large sample of different methods and the complexity of their implementation.

Long-term supported platforms are not chosen accidentally. The main list of technologies used includes C#, the WPF (Windows Presentation Foundation) application platform, a SQLite database that supports dynamic data typing. Due to the type of task, which assumes long-term accumulation of the sample database under consideration, as well as less time for software support.

The giant Raman scattering spectra database allows users to detect the desired spectra from experimental data and compare them with reference spectra.

The main purpose of this system is to reduce the cost of buying a spectra database as well as its use, while being able to support the software for many years. Databases in a particular case make it possible to structure a large amount of actual information, to display information on demand in a representative manner, and to provide a quick and trouble-free access to the necessary elements with aggregation.

Finally, a correlation method with pattern linking was chosen, which has no disadvantages of previous classifiers and has sufficient accuracy at the same time.

The work resulted in a ready-made complete software solution that allows you to solve all the tasks described above. It is important to note that the analysis of various algorithms (neural network, Bayesian the classifier) has been made, allowing to verify effectively the belonging of the reference spectrum to the one under consideration.

References:

1. Sha, M. Y. Surface-Enhanced Raman Scattering Tags for Rapid and Homogeneous Detection of Circulating Tumor Cells in the Presence of Human Whole Blood / M. Y. Sha [et al] // J. Am. Chem. Soc. – 2008. – Vol. 130. – P. 17214–17215.

2. Vo-Dinh, T. Cancer Gene Detection Using Surface-enhanced Raman Scattering (SERS) / T. Vo-Dinh, L. R. Allain, D. L. Stokes // J. Raman Spectrosc. – 2002 – Vol. 33. – P. 511–516.

3. Урядов В.Н., Глущенко Formation of sers-active silver structures on the surface of mesoporous silicon // A. Yu. Panarin [et al.] / Journal of Applied Spectroscopy. – 2009. – Vol. 76. – № 2. – P. 280-287.

4. Aroca, R. Surface-enhanced vibrational spectroscopy/ R. Aroca. – Chichester: J. Wiley, 2006. – 233 p.

5. Formation of sers-active silver structures on the surface of mesoporous silicon // A. Yu. Panarin [et al.] / Journal

6. Ryzhii, M. Monte Carlo modeling of transient effects in resonant–tunneling bipolar transistors / M. Ryzhii // Jpn. J. Appl. Phys. – 1994. – Vol. 36, № 8. – P. 5060–5062.

7. Reyes-Goddard, J. M. Photodiagnosis Using Raman and Surface Enhanced Raman Scattering of Bodily Fluids / J. M. Reyes-Goddard, H. Barr, N. Stone // Photodiag. and Photodyn. Therapy. – 2005. – Vol. 2. – P. 223–233.

8. Farquharson, S. Surface-enhanced Raman Spectral Measurements of 5-Fluorouracil in Saliva / S. Farquharson [et al] // Molecules. – 2008. – Vol. 13. – P. 2608–2627.